Exhibit 300: Capital Asset Summary

Part I: Summary Information And Justification (All Capital Assets)

Section A: Overview & Summary Information

Date Investment First Submitted: 2009-06-30
Date of Last Change to Activities:
Investment Auto Submission Date: 2012-02-16
Date of Last Investment Detail Update: 2012-02-16
Date of Last Exhibit 300A Update: 2012-02-16
Date of Last Revision: 2012-08-28

Agency: 019 - Department of Energy **Bureau:** 20 - Energy Programs

Investment Part Code: 01

Investment Category: 00 - Agency Investments

1. Name of this Investment: PNNL EMSL, High Performance Computer Center Operations and Maintenance - Direct Mission

2. Unique Investment Identifier (UII): 019-000000915

Section B: Investment Detail

1. **Provide a brief summary of the investment, including a brief description of the related benefit to the mission delivery and management support areas, and the primary beneficiary(ies) of the investment. Include an explanation of any dependencies between this investment and other investments.**

The Molecular Science Computing Facility (MSCF) is only one of eight parts of the Environmental Molecular Sciences Laboratory (EMSL), a DOE scientific user facility for molecular-level science located at Pacific Northwest National Laboratory in Richland, WA. EMSL provides more than 60 world-class experimental research instruments, and a high performance computing (HPC) capability & associated data storage to users to enable iteration between theory & experiment to advance DOE Goal 2, Science and Engineering Enterprise. Usage of MSCF s HPC capability remains consistently greater than 97% & requests for time are consistently more than double availability. MSCF is the sole computing facility in the DOE complex that optimizes its HPC for molecular-level environmental sciences computation, & time on the HPC is actively managed to ensure integration with the experimental resources in EMSL. W/o this highly integrated HPC resource within the EMSL facility, the MSCF s more than 200+ users would be unable to quickly verify molecular-level experimental results, thereby significantly slowing publication of findings relevant to DOE missions and making it impossible to iterate between computation & experiment in real-time. Current cloud platforms do not provide sufficient capacity, performance or quality of service for scientific parallel codes needed by EMSL users. MSCF's HPC is one EMSL tool in DOE's efforts to predict the movement and remediation of contaminants at DOE sites, understand &

enhance catalysis and biofuels processing, and investigate the coupling of chemical, biological and physical processes at the molecular level. Time on MSCF s HPC is made available to users from DOE's basic research and applied R&D programs, and to users funded by other Federal agencies (e.g. NSF, NIH, USGS, DOD, EPA). MSCF maintains a steady state operation. Through operations funding to EMSL, the HPC is replaced every 3-4 yrs by leasing commercially available hardware through fixed price contracts in accordance with DOE's Project Management Order, as overseen by the Office of Project Assessment in DOE's Office of Science (SC). In FY 2013 this consolidated investment has been split into two components; O&M for the HPC center and lease for the HPC. The BY13 funding has been distributed accordingly between this investment and PNNL EMSL, High Performance Computer Lease - Direct Mission UII 019-000000133 00-20-01-21-02-00.

2. **How does this investment close in part or in whole any identified performance gap in support of the mission delivery and management support areas? Include an assessment of the program impact if this investment isn't fully funded.**

This investment enables the scientific community to address two of the targeted outcomes under Goal 2, Science and Engineering Enterprise, within the 2011 DOE Strategic Plan. These include: a) "...develop and explore a broad spectrum of new materials that have novel properties, such as catalysis, electrochemical behavior, radiation resistance or strength...," and b) "...apply systems biology approaches...to create viable biofuels processes and greatly increase the understanding of microbes in carbon-dioxide climate balance..." If this investment is not fully funded, then scientists will not be able to iterate between experimental research and computational research to achieve a molecular-level understanding of the environmental and energy challenges facing DOE and the Nation. Usage of MSCF s HPC capability remains consistently greater than 97% & requests for time are consistently more than double availability.

3. **Provide a list of this investment's accomplishments in the prior year (PY), including projects or useful components/project segments completed, new functionality added, or operational efficiency achieved.**

This investment, one of more than 60 scientific capabilities within EMSL, was designed specifically to meet the needs of computational chemistry and bioinformatics in support of experimental investigations aligned with the EMSL mission. The primary compute cluster, a production system named Chinook, exceeded the 97% availability target for FY11 with over 90% of the cycles used for EMSL s science theme users. During FY11, an additional 1.5 petabytes of usable archive space was made available to users, and the response time to address user issues was well below the target of 120 minutes.

4. **Provide a list of planned accomplishments for current year (CY) and budget year (BY).**

In CY12 and BY13, this investment will prepare the facility for, and plan and execute the procurement of a new higher performance midrange HPC system, HPCS-4a. It will continue to operate the existing HPCS-3 (Chinook) HPC system, and augment the tape and disk capacity of the EMSL data archive system. Expected scientific accomplishments include: Develop fundamental catalytic surface characterization simulations for biomass conversion to ethanol using rhodium catalysts. Combine electronic structure computational simulation

with cryogenic NMR experiments to understand photosynthetic energy conversion systems. Use NMR and computational biochemistry to determine conformational changes within an active enzyme/substrate on both sides of the reaction. Develop more efficient fuel cells by simulating molecular-level reactions that could occur at a variety of material interfaces. Establish a fundamental and comprehensive molecular and multi-scale understanding of the influence of complex real-world geochemical environments on the speciation, adsorption, reduction chemistry, and chemical transformation of actinide species, using statistical and quantum mechanical computational chemistry tools. Combine theoretical computation with laser-stimulated desorption measurements of neutral oxygen and zinc atoms on zinc oxide surfaces to understand the mechanisms of radiation damage and scintillating properties of metal oxides.

5. **Provide the date of the Charter establishing the required Integrated Program Team (IPT) for this investment. An IPT must always include, but is not limited to: a qualified fully-dedicated IT program manager, a contract specialist, an information technology specialist, a security specialist and a business process owner before OMB will approve this program investment budget. IT Program Manager, Business Process Owner and Contract Specialist must be Government Employees.**

2007-01-11

Section C: Summary of Funding (Budget Authority for Capital Assets)

1.

Table I.C.1 Summary of Funding

	PY-1 & Prior	PY 2011	CY 2012	BY 2013
Planning Costs:	$2.4	$0.0	$0.0	$0.0
DME (Excluding Planning) Costs:	$29.6	$0.0	$0.0	$0.0
DME (Including Planning) Govt. FTEs:	$0.0	$0.0	$0.0	$0.0
Sub-Total DME (Including Govt. FTE):	$32.0	0	0	0
O & M Costs:	$64.7	$10.1	$9.2	$7.3
O & M Govt. FTEs:	$0.3	$0.0	$0.0	$0.0
Sub-Total O & M Costs (Including Govt. FTE):	$65.0	$10.1	$9.2	$7.3
Total Cost (Including Govt. FTE):	$97.0	$10.1	$9.2	$7.3
Total Govt. FTE costs:	$0.3	0	0	0
# of FTE rep by costs:	4	1	1	1
Total change from prior year final President's Budget ($)		$0.0	$0.0	
Total change from prior year final President's Budget (%)		0.00%	0.00%	

2. If the funding levels have changed from the FY 2012 President's Budget request for PY or CY, briefly explain those changes:

Not changed. Milestones and Summary of Funding table in FY11 and beyond have been modified to re-classify this investment as steady state. This classification has more fidelity, transparency and is consistent with its function as a scientific user facility and data reported with budget narratives.

Section D: Acquisition/Contract Strategy (All Capital Assets)

Table I.D.1 Contracts and Acquisition Strategy

Contract Type	EVM Required	Contracting Agency ID	Procurement Instrument Identifier (PIID)	Indefinite Delivery Vehicle (IDV) Reference ID	IDV Agency ID	Solicitation ID	Ultimate Contract Value ($M)	Type	PBSA ?	Effective Date	Actual or Expected End Date
Awarded	8900	DEAC0576RL01830:572	NA	8900							

2. If earned value is not required or will not be a contract requirement for any of the contracts or task orders above, explain why:
Contract DE-AC05-76RL01830:572 and its extension (same #) represent the Prime Contract for the entire Pacific Northwest National Laboratory (PNNL), of which the EMSL is a part. The values reported there represent that portion of the Prime Contract that funds the MSCF part of the EMSL. The MSCF Project Director submits monthly operational performance reports of the steady state investment to the assigned DOE program manager in BER. These include project cost and performance and earned value statistics when projects are being executed. EVM is implemented on appropriate sub-contracts as required by the Prime Contract.

Exhibit 300B: Performance Measurement Report

Section A: General Information

Date of Last Change to Activities:

Section B: Project Execution Data

Table II.B.1 Projects

Project ID	Project Name	Project Description	Project Start Date	Project Completion Date	Project Lifecycle Cost ($M)
	NONE				

Activity Summary

Roll-up of Information Provided in Lowest Level Child Activities

Project ID	Name	Total Cost of Project Activities ($M)	End Point Schedule Variance (in days)	End Point Schedule Variance (%)	Cost Variance ($M)	Cost Variance (%)	Total Planned Cost ($M)	Count of Activities
NONE								

Key Deliverables

Project Name	Activity Name	Description	Planned Completion Date	Projected Completion Date	Actual Completion Date	Duration (in days)	Schedule Variance (in days)	Schedule Variance (%)
				NONE				

Section C: Operational Data

Table II.C.1 Performance Metrics

Metric Description	Unit of Measure	FEA Performance Measurement Category Mapping	Measurement Condition	Baseline	Target for PY	Actual for PY	Target for CY	Reporting Frequency
Maintain overall response time to customer support requests	Minutes per response	Customer Results - Timeliness and Responsiveness	Under target	120.000000	120.000000	22.000000	120.000000	Monthly
Maintain Chinook utilization in FY12	Node Hours (millions)	Process and Activities - Productivity	Over target	16.900000	16.900000	17.000000	16.900000	Monthly
Maintain Chinook availability in FY12	Percent Availability	Process and Activities - Productivity	Over target	97.000000	97.000000	98.000000	97.000000	Monthly
Increase # of Terabytes available for archive of scientific data.The EMSL data archive will receive tape expansions, making more Terabytes of storage space available than in the previous year.	Terabytes	Technology - Information and Data	Over target	6000.000000	6000.000000	6000.000000	6000.000000	Monthly
Maintain average time a customer ticket is open	Hours per open time	Customer Results - Timeliness and Responsiveness	Under target	24.000000	24.000000	15.000000	24.000000	Monthly